

A theoretical study of the cluster glass-Kondo-magnetic disordered alloys

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Abstract

The physics of disordered alloys, such as typically the well known case of CeNi_{1-x}Cu_x alloys, showing an interplay among the Kondo effect, the spin glass state and a magnetic order, has been studied firstly within an average description like in the Sherrington-Kirkpatrick model. Recently, a theoretical model [1] involving a more local description of the intersite interaction has been proposed to describe the phase diagram of CeNi_{1-x}Cu_x. This alloy is an example of the complex interplay between Kondo effect and frustration in which there is in particular the onset of a cluster-glass state. Although the model given in Ref. [1] has reproduced the different phases relatively well, it is not able to describe the cluster-glass state. We study here the competition between the Kondo effect and a cluster glass phase within a Kondo Lattice model with an inter-cluster random Gaussian interaction. The inter-cluster term is treated within the cluster mean-field theory for spin glasses [2], while, inside the cluster, an exact diagonalisation is performed including inter-site ferromagnetic and intra-site Kondo interactions. The cluster glass order parameters and the Kondo correlation function are obtained for different values of the cluster size, the intra-cluster ferromagnetic coupling and the Kondo intra-site coupling. We obtain, for instance, that the increase of the Kondo coupling tends to destroy the cluster glass phase.

1 Introduction

The properties of many cerium or uranium compounds are well described by the Kondo-lattice model, in which there is a strong competition between the Kondo effect on each site and the Ruderman-Kittel-Yosida-Kasuya (RKKY) interaction between magnetic atoms at different sites. On the other hand, it is now quite clear that the interplay between disorder and electronic correlations in these systems produces a new physics such as the presence of Non-Fermi liquid behaviour [3, 4, 5] or percolative process in the magnetic states similar to manganites [6].

An example of the percolative scenario can be found in $CeNi_{1-x}Cu_x$ [7]. This particular alloy presents a quite complex phase diagram as long as the doping of Ni increases. In the range of doping $0.6 < x < 0.3$, the μ SR results indicate formation of

clusters below a characteristic temperature T^* . On the other hand, the ac-susceptibility (χ_{ac}) shows the presence of a glassy ordering below a freezing temperature T_f ($T_f < T^*$). In this sense, this particular state can be characterized as a Cluster Glass (CG) state. Finally, it has been found an inhomogeneous ferromagnetic (IFM) order from neutron diffraction at much lower temperature. However, there is no clear indication of a Curie temperature T_c from χ_{ac} and C_p measurements. Therefore, it is possible to speculate that the evolution from CG state to the IFM order can be obtained by the percolation of the frozen clusters. One important experimental evidence supporting such scenario has been the behaviour of the hysteresis loops for $CeNi_{0.6}Cu_{0.4}$ at $T = 100$ mK which display discrete jumps of the magnetization.

From the theoretical point of view, a model has been proposed to explain the presence of frustration in the global phase diagram of $CeNi_{1-x}Cu_x$. The model is a Kondo Lattice with an additional Ising intersite interaction between localized spins called here Kondo-Ising Lattice (KIL) model [9]. The important point is that disorder can be introduced in the KIL model by choosing, for instance, the coupling J_{ij} between the localized spins as a Gaussian random variable (see for example, the Sherrington-Kirkpatrick (SK) model [10]). The results have shown that it is possible to construct a mean field solution of the KIL model, where it is found a spin glass SG solution as well as a Kondo regime [9]. This approach has been extended to include a ferromagnetic (FM) solution [11] by displacing the Gaussian distribution from the origin to J_0 . This procedure has allowed to introduce the usual magnetization as a new order parameter. As a result, a global phase diagram temperature *versus* J_K (the strength of Kondo coupling) has been obtained displaying a SG phase, an additional FM one and a Kondo regime. However, the sequence of phase transitions when the temperature is decreased (for a constant J_K) is not in agreement to the experimental findings. On the contrary, the FM solution appears at higher temperature than the SG one. Moreover, there is no percolation process. The results also show a conventional phase transitions in which there is, for instance, a clear Curie temperature T_c . It is also important to remark that the usual FM order parameter included in this particular approach is not able to capture the complexity of the experimental IFM ordering.

Recently, a new approach has been proposed replacing the random Gaussian J_{ij} in Eq. (1) for random site model in which $J_{ij} = \sum_{\mu=1}^p \xi_i^\mu \xi_j^\mu$, where ξ_i^μ are random variables which follow the distribution $P(\xi_i^\mu) = 1/2\delta_{\xi_i^\mu, 1/2} - 1/2\delta_{\xi_i^\mu, -1/2}$ [12]. In fact, this particular choice of J_{ij} can allow the interpolation from weak to strong frustration regimes. This model improves the previous SK-based model in two directions: first it gives a better possible description of the experimental IFM ordering and second it yields a disordered ferromagnetic phase below the spin glass one in better agreement with the experiment. However, it is still necessary further theoretical improvements to describe the magnetic clusters in $CeNi_{1-x}Cu_x$.

The presence of the cluster glass is a clear indicative that the frustration present in the intermediated doping of $CeNi_{1-x}Cu_x$ can not be described by a conventional spin glass. One possible improvement to the original KIL model would be to reformulate the intersite random interaction using cluster of spins instead of canonical spins. In fact, in a earlier work [2], the classical cluster glass problem has been studied in a mean field level. The model used is composed, basically, by a intracluster ferromagnetic coupling and a intercluster Gaussian random coupling. This kind of approach seems adequate to be implemented to study the competition between Kondo effect and cluster glass within the approach of Ref. [9]. Therefore, cluster of spins could be introduced in the original KIL model [9] by replacing the intersite random Gaussian term by intracluster

and intercluster terms similar to Ref. [2].

The aim of the present work is to study competition between Kondo effect and cluster glass. In view of the discussion in the previous paragraph, we use the following model (called here Kondo Lattice Cluster Glass (KLCG)) to accomplish that study:

$$H = \sum_{a=1}^{N_{cl}} \sum_{i=1}^{n_s} \epsilon_0 \sum_{\sigma=\uparrow\downarrow} \hat{n}_{i\sigma a}^f - J_0 \sum_{a=1}^{N_{cl}} \sum_{i<j}^{n_s} \hat{S}_{ia}^z \hat{S}_{ja}^z + \sum_a \sum_{i,j}^{N_{cl}} t_{ij}^{aa} d_{i\sigma a}^\dagger d_{j\sigma a} \quad (1)$$

$$+ J_k \sum_{a=1}^{N_{cl}} \sum_{i=1}^{n_s} \left(\hat{S}_{ia}^+ s_{ia}^- + \hat{S}_{ia}^- s_{ia}^+ \right) - \sum_{a<b}^{N_{cl}} J_{ab} \hat{S}_a^z \hat{S}_b^z$$

where intercluster coupling J_{ab} is a random variable as the Sherrington-Kirkpatrick model

$$P(J_{ab}) = e^{-J_{ab}^2 (N_{cl}/32J^2)} \sqrt{\frac{N_{cl}}{32\pi J^2}} \quad (2)$$

with $N = N_{cl} * n_s$, where N_{cl} and n_s are the number of cluster and the number of spin in each cluster, respectively. The hopping t_{ij}^{aa} is only inside the cluster. The indices (a, b) refer to clusters while (i, j) indicates spins inside a cluster. So, $S_{ia}^+ = f_{ia\uparrow}^\dagger f_{ia\downarrow}$, $s_{ia}^- = d_{ia\downarrow}^\dagger f_{ia\uparrow}$ and

$$\hat{S}_a^z = \sum_{i=1}^{n_s} \sum_{\sigma=\uparrow\downarrow} \sigma f_{i\sigma a}^\dagger \hat{f}_{i\sigma a} = \sum_{i=1}^{n_s} \hat{S}_{ia}^z \quad (3)$$

$$\hat{S}_{ia}^z = \sum_{\sigma=\uparrow\downarrow} \sigma f_{i\sigma a}^\dagger \hat{f}_{i\sigma a} \quad (4)$$

The problem can be treated within the formalism of integral functional where the spin operators are given by bilinear combinations of Grassmann fields. It should be remarked that disorder is introduced only in the intercluster random Gaussian interaction J_{ab} . Nonetheless, the thermodynamics for this particular situation is also obtained using the replica method. So,

$$\beta F = -\frac{1}{N} \lim_{n \rightarrow 0} \frac{\langle Z^n \rangle_{J_{ab}} - 1}{n}. \quad (5)$$

The procedure to deal with the disorder follows closely the usual fermionic spin glass (see for instance [13]). The problem is treated within the static approximation with order parameters $q_{\alpha\beta}$ ($\alpha \neq \beta$) and $q_{\alpha\alpha}$ being introduced by a Hubbard-Stratonovich transformation. Then, replica symmetry is assumed $q = q_{\alpha\beta}$ and $p = q_{\alpha\alpha}$. The main difference is that, in the present approach, these order parameters describe a glassy ordering among cluster instead of canonical spins. The details of the calculations will be shown elsewhere [14].

The free energy is

$$\beta F = \frac{(\beta J)^2}{2} p^2 - \frac{(\beta J)^2}{2} q^2 - \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} e^{-\frac{z^2}{2}} \ln \left[\int_{-\infty}^{+\infty} \frac{d\xi}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}} Z_{eff}^c \right] \quad (6)$$

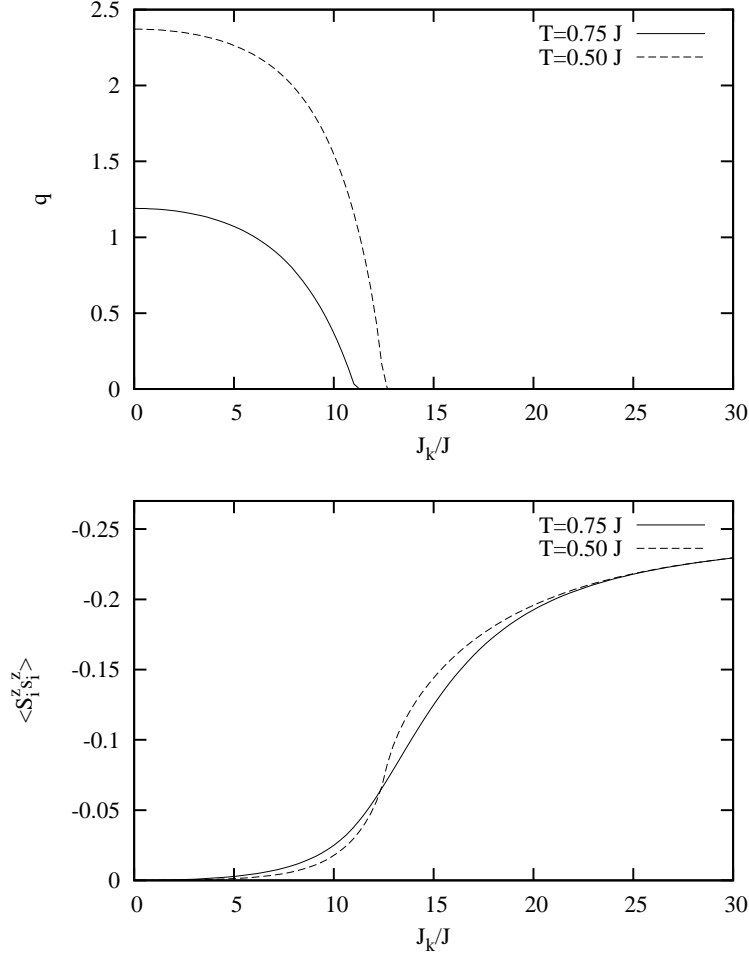


Figure 1: Spin glass order parameter and correlation function $\langle S_i^z S_i^z \rangle$ versus J_k/J for $n_s = 2$ and $J_0/J = 1$. The dashed lines are results at temperature $T = 0.50J$ and the full lines correspond to results at $T = 0.75J$.

and

$$Z_{eff}^c = \int D(\varphi^* \varphi) D(\psi^* \psi) e^{A_{eff}} \quad (7)$$

That is equivalent to diagonalize the following Hamiltonian:

$$H_{eff} = \sum_{\sigma} \left[\sum_{i=1}^{n_s} \epsilon_0 \hat{n}_{i\sigma} + \sum_{i,j}^{n_s} t_{ij} \hat{d}_{i\sigma}^{\dagger} d_{j\sigma} \right] + J_k \sum_{i=1}^{n_s} \left[\hat{S}_i^{\dagger} s_i^{-} + \hat{S}_i^{-} s_i^{+} \right] - J_0 \sum_{i < j}^{n_s} \hat{S}_i^z \hat{S}_j^z + 2h(p, q) \sum_{j=1}^{n_s} \hat{S}_j^z \quad (8)$$

where $h(p, q)$ is given as

$$h(p, q) = \beta J \sqrt{2(p-q)} \xi + \sqrt{2q} z. \quad (9)$$

Then, in the effective problem, $h(p, q)$ appears as a random external field applied in the cluster which depends on the clusters glass order parameters q and p . Therefore, to obtain any information in this problem, it is necessary to diagonalize the Hamiltonian H_{eff} given in Eq. (8) and, simultaneously, to solve the saddle point equations for q and p .

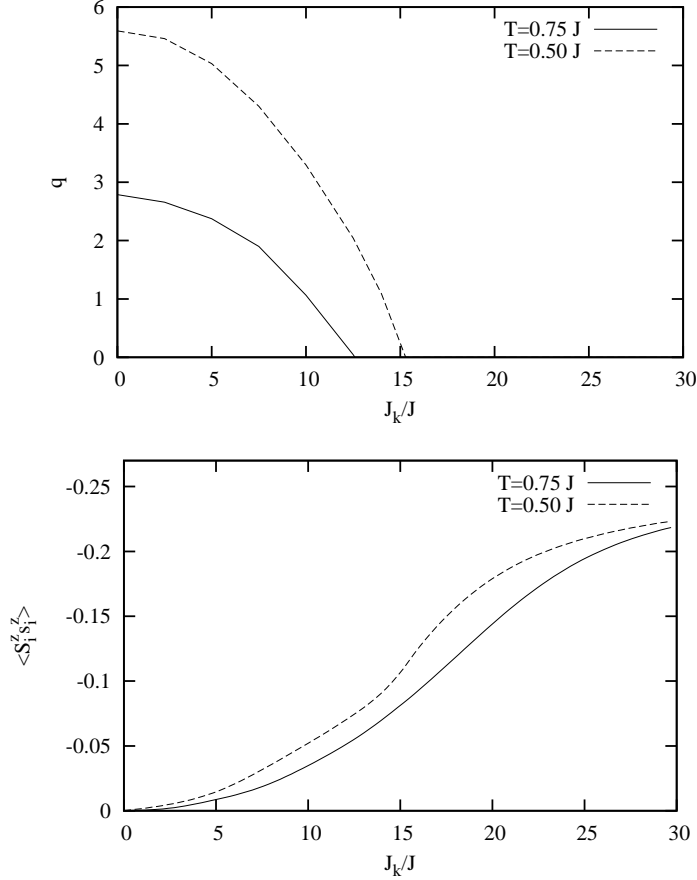


Figure 2: Spin glass order parameter and correlation function $\langle S_i^z S_i^z \rangle$ versus J_k/J for $n_s = 3$ and $J_0/J = 1$. The dashed lines are results at temperature $T = 0.50J$ and the full lines correspond to results at $T = 0.75J$.

The behaviour of the cluster glass order parameters q and the Kondo correlation function $\langle S_i^z S_i^z \rangle$ are displayed in Figs. 1-2 as a function of the Kondo coupling J_K for two values of temperature T while the intracluster ferromagnetic coupling is kept constant $J_0 = J$ (J is defined in Eq. (2)). The size of the clusters also assumes two values, $n_s = 2$ and 3. In Fig. 1, the results for $n_s = 2$ show that, when J_k increases, the cluster glass order parameters q decreases. For $T = 0.75J$ and $T = 0.5J$, the cluster glass phase are destroyed for $J_K \approx 11J$ and $J_K \approx 13J$, respectively. While q decreases, $\langle S_i^z S_i^z \rangle$ enhances which means that the Kondo effect inside the cluster becomes increasingly

important. The combined behaviour of q and $\langle S_i^z S_i^z \rangle$ would indicate that increase of the Kondo effect inside the cluster is related to the destruction of the cluster glass phase. For $n_s = 3$, the scenario described previously is preserved with q decreasing and $\langle S_i^z S_i^z \rangle$ increasing. However, q vanishes for larger values of J_K as compared with the case $n_s = 2$, particularly, for $T = 0.5J$. That result would suggest that the cluster glass phase becomes more robust with the increase of n_s .

To conclude, in the present work we have studied the competition between cluster glass phase and Kondo effect using the Kondo Lattice Cluster Glass model defined in Eq. (1). The intercluster disorder problem is treated using the usual mean field procedure for fermionic spin glasses. Therefore, the original problem is transformed in an effective one in which there is a random external field applied on the cluster. Finally, it is used exactly diagonalization to solve the cluster. The results indicate that, when J_K increases, the Kondo correlation function $\langle S_i^z S_i^z \rangle$ also increases. Simultaneously, the cluster glass phase is destroyed. These results suggest that this approach could be used to study the behaviour of the $CeNi_{1-x}Cu_x$. However, as discussed previously, the frustration in cited physical system can not be described in terms of a random Gaussian coupling. It would be better described by a coupling used in Ref. [1]. This approach is under current investigation.

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